### Asymptotic Behavior of Lévy Walks

#### BACHELOR THESIS

for attaining the academic grade of Master of Science (M. Sc.) in the field of Physics



submitted to Mathematisch-Naturwissenschaftliche Fakultät I Institut für Physik Humboldt-Universität zu Berlin

> by Marius Bothe born 23. February 1995

#### Supervising tutors:

- 1. Prof. Dr. Igor Sokolov
- 2. Dr. Michael Zaks

Submitted on: XXXXXXXXXX

# Contents

1	Intr	roduction	1
2	The	eoretical Background	2
	2.1	The model	2
		2.1.1 Lévy walks	2
		2.1.2 Generalized Lévy walks	
	2.2		
		2.2.1 Continuous time random walks	
		2.2.2 Space-time coupled continuous time random walks	
3	Methodology		
	3.1	Calculating the mean squared displacement	12
	3.2	Finding the probability density function	
	3.3	Numerical simulation of the model	
4	Analytical Calculations		15
5	Res	Results and Discussion	
6	Conclusions		17

# 1. Introduction

hat er das jetzt geaendert?

### 2. Theoretical Background

#### 2.1 The model

#### 2.1.1 Lévy walks

The original motivation for the creation of the Lévy walk model goes back to the work of Richardson in 1926 [1], who studied the motion of particles in the turbulent flow of the atmosphere. Such a system contains jets and eddies that affect the behavior of the particle and lead to anomalous diffusion. In particular Richardson found that the mean squared displacement (MSD) of the particle scales with the third power of the time, i.e.

$$\langle \mathbf{x}^2 \rangle(t) \propto t^3,$$
 (2.1)

which is known as the Richardson regime.

There were several attempts to find a random walk model that replicates this behavior. These attempts found that power-law models were particularly suitable for describing superdiffusion <sup>1</sup> which lead to the creation of the Lévy flight model: In this model the walker jumps instantaneously in a random direction with a jump length drawn from a distribution  $g(|\mathbf{x}|)$ . He now waits at the turning point for the duration of the waiting time, which is drawn from the distribution  $\psi(t)$  and then performs a new jump in another direction, as can be seen in figure (2.1). Both the waiting time and the jump length distributions are power-laws, meaning for large arguments they take the form

$$\psi(t) \propto t^{-1-\gamma}, \qquad g(|\mathbf{x}|) \propto |\mathbf{x}|^{-1-\beta}, \qquad \gamma, \beta > 0.$$
 (2.2)

However the Lévy flight model has a major drawback: Since the jumps happen instantaneously it has an infinite propagation speed, which causes its MSD and all higher moments to diverge [2].

Therefore the Lévy walk model was developed by Shlesinger, Klafter and West [3]. Here the walker no longer waits at the turning points, but his jumps now have a finite duration, turning them into steps. The step duration is coupled to the length of the step and prevents the infinite propagation speed that caused problems with the Lévy flights, which is illustrated in figure 2.1.

meaning diffusion where  $\langle \mathbf{x}^2 \rangle(t) \propto t^{1+\alpha}$ ,  $\alpha > 0$ 

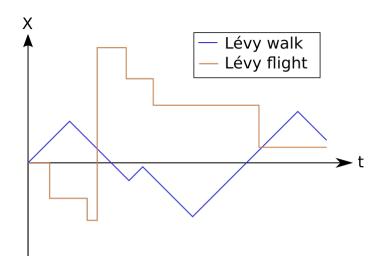


Figure 2.1: Comparison between the trajectories of the one dimensional Lévy flight and Lévy walk (for  $\nu = 1$ ). Note that the jump length of the Lévy flight is independent of the waiting time.

The path of a walker in the new model is now described by a series of step durations  $t_1, t_2, ...$  which are drawn from the power-law distribution

$$\psi(t_i) = \frac{\gamma}{t_0} \frac{1}{(1 + t_i/t_0)^{\gamma + 1}}.$$
(2.3)

Here the parameter  $\gamma > 0$  governs the width of the distribution and  $t_0$  is the timescale of a step. These step durations are associated with their respective steps vectors  $\mathbf{x}_1, \mathbf{x}_2, ...$ , whose direction is chosen randomly. By partially summing up the step durations and the step lengths one obtains the turning times  $T_n$  and the turning points  $\mathbf{X}_n$  respectively:

$$T_n = \sum_{j=1}^n t_j, \qquad \mathbf{X} = \sum_{j=1}^n \mathbf{x}_j \tag{2.4}$$

The walker is now being observed at the observation time t: Let the last turning time before t be  $T_n = \max\{T_i|T_i \leq t\}$ , then the distance covered from the last turning point is given by

$$|\mathbf{x}_{n+1}| = c(t_{n+1})^{\nu-1}(t-T_n),$$
 (2.5)

where c is a constant with dimension  $[st^{-\nu}]$ . The speed

$$v = \frac{\partial}{\partial t} |\mathbf{x}_{n+1}| = c(t_{n+1})^{\nu-1}$$
(2.6)

is therefore constant during the entire step but depends on the step duration  $t_{n+1}$ , where the parameter  $\nu > 0$  governs this dependence.

For any completed step we can now write down the joint probability to make a step of length  $|\mathbf{x}|$  and duration t:

$$\psi(\mathbf{x},t) = \frac{\gamma}{t_0} \frac{1}{(1+t/t_0)^{\gamma+1}} \frac{\delta(|\mathbf{x}| - ct^{\nu})}{|\mathbf{x}|^{d-1} |S^{d-1}|}.$$
 (2.7)

Here d is the spatial dimension of the process and  $|S^{d-1}|$  is the surface area of a d-dimensional unit ball. Note that both the step duration distribution and the joint distribution are denoted by  $\psi$ , but their arguments are different. In conclusion we have a model that is governed by two parameters,  $\nu$  and  $\gamma$  and can produce different kinds of anomalous diffusion.

Because of this versatility the Lévy walk model is used to describe a variety of systems: Besides the application in turbulent systems for which the model was originally invented it finds application in field like biology, where the special case of fixed velocities ( $\nu=1$ ) is used to approximate the motion of E. coli bacteria, who move with the help of microscopic flagella. These flagella either rotate in a synchronized manner, which leads to long stretches of relatively fast movement, or unsynchronized, which leads to a tumbling motion in which the bacterium changes its direction. The resulting motion was found to follow a power-law distribution with parameter  $\gamma=1.2$  [4]

However it was found recently in [5] that the MSD of the model is actually divergent for certain values of its parameters, a fact that had previously gone unnoticed for the three decades of the models existence. The divergence can be seen directly when one writes down the contribution to the second moment of the distribution from the trajectories, that consist only of a single step longer than the observation, i.e. where the particle never stops:

 $\langle \mathbf{x}^2 \rangle(t) \ge \int_{\mathbb{R}^d} \int_t^\infty |\mathbf{x}|^2 (t') \psi(\mathbf{x}, t') dt' d^d x$  (2.8)

$$= \frac{\gamma}{t_0} \int_0^\infty \int_t^\infty |\mathbf{x}|^2 (t') \frac{1}{(1 + t'/t_0)^{\gamma + 1}} \delta(|\mathbf{x}| - c(t')^{\nu - 1} t) dt' d|\mathbf{x}|$$
 (2.9)

$$= \frac{\gamma t^2}{t_0} \int_t^\infty \frac{c^2(t')^{2\nu - 2}}{(1 + t'/t_0)^{\gamma + 1}} dt'. \tag{2.10}$$

The integrand is proportional to  $(t')^{2\nu-\gamma-3}$ , therefore the integral will diverge at infinity whenever  $2\nu \geq \gamma + 2$  holds. This includes the parameter region where the Richardson regime was expected, so the model that was essentially invented to cure the divergence in the description of the Richardson regime turns out to be divergent itself. In order to remedy this, a more general model model is necessary.

#### 2.1.2 Generalized Lévy walks

Because the divergence of the second moment is caused by very long steps that result in arbitrarily high velocities throughout the entire step, a solution can be found by letting the particle start with a lower initial speed and compensating for the slower start by accelerating it throughout the step, so that it catches up with its constant velocity counterpart at the end of the step.

There are indeed some models that describe particles under acceleration [6,7] that

more examples: light
scattering,
chaotic
Hamiltonian
systems

Say something about ballistic cone?

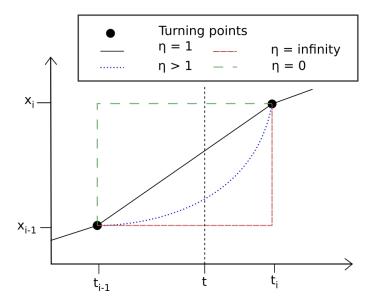


Figure 2.2: Comparison of the walkers motion for different values of  $\eta$ : The trajectories and turning points remain the same, but the position measured at time t varies. For  $\eta = 1$  the walker moves with constant speed and has some non-linear time dependence for  $\eta > 1$ . In the limits  $\eta = 0$  and  $\eta = \infty$  we replicate the time-coupled Lévy flight, where the two limits correspond to the walker jumping first and then waiting or waiting first and then jumping.

are similar to the Drude model for solids. There it is shown that the MSD exists in the regime where one would expect the Richardson law.

Furthermore in the supplementary material of [5] a model is presented that introduces an additional parameter,  $\eta$ , that allows one to interpolate between the original Lévy model and the Drude like sheme. It is this model, which I will call generalized Lévy walk model, that I will investigate in this thesis.

The generalized model uses the same distribution of step durations as the previous model (??), but the position between two turning points is calculated differently. Instead of a linear time dependence we now have a dependence on the new parameter  $\eta$  for the displacement in the (n+1)th step:

$$|\mathbf{x}_{n+1}| = c(t_{n+1})^{\nu-\eta} (t - T_n)^{\eta}.$$
 (2.11)

Therefore the particle moves in general with a non-constant speed

$$v = c\eta(t_{n+1})^{\nu-\eta}(t - T_n)^{\eta-1}.$$
(2.12)

We note, that this changes neither the turning points, nor the turning times and the distribution of completed steps is still given by

$$\psi(\mathbf{x},t) = \frac{\gamma}{t_0} \frac{1}{(1+t/t_0)^{\gamma+1}} \frac{\delta(|\mathbf{x}| - ct^{\nu})}{|\mathbf{x}|^{d-1} |S^{d-1}|}.$$
 (2.13)

However the position in between the points now depends a on  $\eta$ , as illustrated in figure (2.2). This affects the last incomplete steps of the walk, which we have seen

to be responsible for the divergence in the original model.

To summarize, the generalized model now depends on three parameters:  $\nu$  determines how the step length of the walker depends on the step durations,  $\eta$  governs the acceleration in between the turning points and  $\gamma$  describes the width of the waiting time distribution. The value of  $\gamma$  has a major influence on the general properties of the model: It determines the power law of  $\psi(t)$ , such that for  $\gamma < 2$  the mean squared step duration diverges and therefore the distribution of culminated duration is no longer subject to the central limit theorem, which states that the distribution of a sum of independent identically distributed random variables with finite variance converges towards a normal distribution.

Therefore the distribution of the sum of waiting times, and by extension the probability distribution function (PDF) of the walk, do not converge to a Gaussian. Instead it was shown by Paul Lévy that in this case the distribution of the sum of the variables converges to one of the so called Lévy alpha stable distributions [2], which is the statement of the generalized central limit theorem. It is this close relation to Lévy distributions that gave the Lévy flights and later the Lévy walks their name.

A second important quality of the Lévy walk model in general and the generalized model in particular is that it is a semi-Markov process. A process is considered Markov if the behavior of the walker after a point in time  $t_0$  only depends on its position and velocity at  $t_0$ , not on its history. For a continuous time random walk (CTRW), for which Lévy walks are an example of, this is usually not the case, as information about the last step, i.e. how long the walker is already moving, is important for predicting the future behavior (with the exception of Gaussian step distributions). However in our case this memory only extends to the last previous step, and the process is renewed at every turning point, therefore it is semi-Markov [2]. Since the path of the walker is dependent on its behavior prior to the beginning of observation it is of great interest to capture this dependence through suitable initial distributions. This was investigated for similar models in [8,9] and in this thesis the distribution of the first turning point  $F(x,t|t_a)$  conditioned on the process aging for a time  $t_a$  is of major importance, as it is needed to calculate the MSD of the aged walk.

A third related property is weak ergodicity breaking in CTRWs. A process breaks ergodicity if its time averages and ensemble averages do not converge to the same values, usually because the trajectory of the solution observed in the time average can not reach the entire phase space, thus giving it only a partial sample. However in the case of weak ergodicity breaking the particle is able to reach the entire phase space, but the time to do this is on the same scale or larger then the total observation time, which means it does not converge reliably to the same value. Ergodicity breaking is of great interest for the theoretical as well as the experimental community as it determines what results we can expect from different kinds of measurements. Power law distributions as used in Lévy process are closely connected to weak ergodicity breaking, as their typical timescale for reaching a convergent average is divergent in subdiffusive regimes [10], and this behavior has been studied for example in [5,11].

While this thesis will not investigate the ergodicity breaking of the new model explicitly, this property is connected to the aged behavior of the walk, which is computed for the MSD All averages are understood to be ensemble averages throughout the thesis.

get
first
hand
source(s)
for
this

#### 2.2 Theory of random walks

In this chapter I will briefly cover some of the main results of the theory of random walks that are used in this thesis. A more detailed description can be found in [12].

#### 2.2.1 Continuous time random walks

#### Mean number of steps

The mean number of steps taken in a walk,  $\langle n \rangle(t)$ , gives an estimate for how fast a walker reaches the regime of asymptotic behavior that is calculated in this thesis. It is therefore important for the comparison of analytical results with numerical simulations.

To derive a general expression for  $\langle n \rangle(t)$  it is necessary to introduce three auxiliary quantities: The survival probability  $\Psi(t)$  describes the chance of a time stretch to last longer than t and can be written as

$$\Psi(t) = \int_{t}^{\infty} \psi(t')dt', \qquad (2.14)$$

where  $\psi(t)$  is the distribution of time stretches. The Laplace transform of such an integral is known and results in

$$\Psi(s) = \frac{1 - \psi(s)}{s}.\tag{2.15}$$

Additionally we need the probability of starting the n-th step at time t, denoted by  $\psi_n(t)$ . It obeys the recursion relation

$$\psi_n(t) = \int_0^t \psi_{n-1}(t')\psi(t-t')dt', \qquad (2.16)$$

Using the convolution property of the Laplace transform (2.29) and induction we find in the Laplace domain:

$$\psi_n(s) = \psi^n(s). \tag{2.17}$$

These two quantities allow us to write down the probability of being in the n-th step at time t,  $\chi(t)$ , i.e. the probability of having started the n-th step at time t' and this step lasting longer than t - t':

$$\chi_n(t) = \int_0^t \psi_n(t') \Psi(t - t') dt'.$$
 (2.18)

Going into the Laplace domain and using results (2.15) and (2.17) we arrive at

$$\chi_n(s) = \psi_n(s)\Psi(s) = \psi^n(s)\frac{1 - \psi(s)}{s}.$$
 (2.19)

The desired mean number of steps can now be expressed as the sum over the  $\chi_n$ :

$$\langle n \rangle(t) = \sum_{n=0}^{\infty} n \chi_n(t)$$
 (2.20)

which yields a closed expression in the Laplace domain:

$$\langle n \rangle(s) = \frac{1 - \psi(s)}{s} \sum_{n=0}^{\infty} n \psi^n(s)$$
 (2.21)

$$= \frac{\psi(s)}{s(1 - \psi(s))}. (2.22)$$

see
how
it
depends
on
existence
of
first

mo-

#### 2.2.2 Space-time coupled continuous time random walks

For a space-time coupled CTRW such as the Lévy walk a each step is determined by a joint distribution of both the step duration t and the step distance  $\mathbf{x}$ , where the coupling between space and time is introduced by one being conditioned on the other:

duction from previ-

ous

ter

chap-

smooth

in-

tro-

$$\psi(\mathbf{x},t) = \psi(t)f(\mathbf{x}|t). \tag{2.23}$$

We are now interested in the distribution of completed steps C(x,t), which is the probability density that a particle starting at  $\mathbf{x}=0$ , t=0 reaches a turning point at time t and position  $\mathbf{x}$  after an arbitrary number of steps in between.

A transport equation can be written down for C(x,t) [12], which reads

$$C(\mathbf{x},t) = \int_{-\infty}^{\infty} d^d \mathbf{x}' \int_0^t dt' C(\mathbf{x}',t') \ \psi(\mathbf{x} - \mathbf{x}',t - t') + \delta(t)\delta(\mathbf{x}). \tag{2.24}$$

The two terms on the right hand side express two different contributions to the probability of finding a turning point at  $(t, \mathbf{x})$ : The first term is a convolution integral in  $\mathbf{x}'$  and t'. It expresses the tautology that there will be a turning point at  $(\mathbf{x}, t)$  exactly when there has been a turning point at the primed coordinates  $(\mathbf{x}', t')$  and the particle performed a jump with displacement  $\mathbf{x} - \mathbf{x}'$  and duration t - t' from  $(\mathbf{x}', t')$  to  $(\mathbf{x}, t)$ .

The second term just enforces that by definition of the density we will find the particle at the origin at the beginning of observation.

To evaluate this integral equation it is useful to go to the Fourier Laplace domain, where the transformations are defined as follows:

The Laplace transform of a function f(t) is defined as the integral

$$\mathcal{L}\left\{f(t), s\right\} = f(s) = \int_0^\infty e^{-st} f(t) dt. \tag{2.25}$$

Note that the distinction between the function and its transform is only made in the argument of the function, which is either t or s.

The Laplace transform is unique up to a set of points with Lebesgue measure zero and can be inverted via the Bromwich integral

$$\mathcal{L}^{-1}\{f(s),t\} = f(t) = \frac{1}{2\pi i} \int_{-i\infty+c}^{+i\infty+c} e^{st} f(s) ds, \tag{2.26}$$

where  $c \in \mathbb{R}$  is chosen such that f(s) exists on the contour.

For Fourier transforms I use the variables  $\mathbf{x} \leftrightarrow \mathbf{k}$ , with the distinction between the function and its transform being made only via the argument. It is defined as

 $\mathcal{F}\left\{f(\mathbf{x}),\mathbf{k}\right\} = f(\mathbf{k}) = \int_{\mathbb{R}^d} e^{i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}) d^d x, \qquad (2.27)$ 

with inverse

 $\mathcal{F}^{-1}\left\{f(\mathbf{k}), \mathbf{x}\right\} = f(\mathbf{x}) = \frac{1}{2\pi} \int_{\mathbb{R}^d} e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{k}) d^d k, \qquad (2.28)$ 

move this to the first place I am using

it

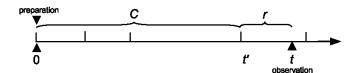


Figure 2.3: Illustration of the path of a Lévy walker on the time axis. Each tick on the line represents a turning time. The walker starts at t = 0 and is observed at time t during a final incomplete step described by the distribution  $r(\mathbf{x}, t)$  after it has completed a series of steps, which is described by  $C(\mathbf{x}, t)$ .

where the normalization factor  $\frac{1}{2\pi}$  is kept in the inverse transform.

A useful property of the Fourier and the Laplace transform is that they turn convolutions of functions into simple products. In particular:

$$\mathcal{L}\left\{\int_0^t f(t')g(t-t')dt', s\right\} = f(s)g(s), \tag{2.29}$$

and

$$\mathcal{F}\left\{ \int_{\mathbb{R}^d} f(\mathbf{x}') g(\mathbf{x} - \mathbf{x}') d^d x', \mathbf{k} \right\} = f(\mathbf{k}) g(\mathbf{k})$$
 (2.30)

Applying this to the integral equation 2.24 we obtain

$$C(\mathbf{k}, s) = C(\mathbf{k}, s) \ \psi(\mathbf{k}, s) + 1 \tag{2.31}$$

and therefore

$$C(\mathbf{k}, s) = \frac{1}{1 - \psi(\mathbf{k}, s)} \tag{2.32}$$

Our next goal is to use this result to write down an expression for the probability distribution of the ordinary, meaning non-aged, Lévy walk  $p(\mathbf{x}|t)$ . It describes the probability of finding the walker at  $\mathbf{x}$  given that it is observed at time t, where it can either be at a turning point or in motion, as illustrated in figure (2.3).

In order to write down a transport equation for  $p(\mathbf{x}|t)$  we need to introduce the probability density for the rest of the walk after the last turning point, denoted by  $r(\mathbf{x}|t)^2$ . As shown in figure (2.3)  $r(\mathbf{x}|t)$  describes the probability of the walker being displaced by the vector  $\mathbf{x}$  after a given time t during a step whose total duration is larger or equal to t:

$$r(\mathbf{x}|t) = \delta(\mathbf{x} - \mathbf{x}'(t'=t)) \int_{t}^{\infty} \psi(\mathbf{x}', t') dt'.$$
 (2.33)

<sup>&</sup>lt;sup>2</sup> Throughout the thesis I will use capital letters for probability densities that depend jointly on space and time, like  $C(\mathbf{x},t)$  and lower case letters for densities that depend only on space and are conditioned on time, like  $r(\mathbf{x}|t)$ . Note that the former have dimension  $[L^{-d}t^{-1}]$ , while the latter have dimension  $[L_{-d}]$ .

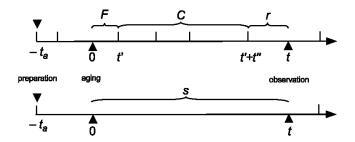


Figure 2.4: Illustration of an aged Lévy walk on the time axis. Each tick on the line represents a turning time. The walker starts at  $-t_a$  and observation begins at t = 0. The upper picture shows the case where the first turning time t' is smaller than the observation time t, described by F. From here it performs a series of completed steps and a final incomplete step as in the ordinary case. The lower picture shows the case that the first turning point is after the end of observation, i.e. the walker never turns during observation. The probability density of this event is given by s.

With this expression for  $r(\mathbf{x}|t)$  we can now write down  $p(\mathbf{x}|t)$  as a convolution of  $r(\mathbf{x}|t)$  and  $C(\mathbf{x},t)$ 

$$p(\mathbf{x}|t) = \int_{\mathbb{R}^d} \int_0^t C(\mathbf{x}', t') r(\mathbf{x} - \mathbf{x}'|t - t') dt' d^d x', \qquad (2.34)$$

which describes the particle starting at the origin, performing a series of completed steps ending at  $\mathbf{x}'$  and then performing a final, incomplete step that leaves it at position  $\mathbf{x}$  at observation time t.

We now use the convolution properties of the Fourier and the Laplace transform, equations (2.30) and (2.29), to obtain

$$p(\mathbf{k}|s) = C(\mathbf{k}, s)r(\mathbf{k}|s). \tag{2.35}$$

Substituting for  $C(\mathbf{k}, s)$  with formula (2.32) yields

$$p(\mathbf{k}|s) = \frac{r(\mathbf{k}|s)}{1 - \psi(\mathbf{k}, s)},\tag{2.36}$$

which gives us an algebraic equation for the PDF in the Fourier Laplace domain, that depends only on the transforms of the step probability density and its time integral. This is a key result for the treatment of space-time coupled CTRW and will be useful for the analytical investigation into the PDF later on.

A slightly more complicated approach is needed when aging effects are considered. In this case the walker has already moved for the duration of the aging time  $t_a$  before the observation begins, which is illustrated in figure (2.4).

At the beginning of observation, which is set to t = 0 and  $\mathbf{x} = 0$ , the walker will already be in motion and has its first observed turning point some time after the beginning of observation, where we denote the probability of this turning point being at  $\mathbf{x}'$  at time t' with  $F(\mathbf{x}', t'|t_a)$ .

Alternatively the walker can also perform a step so long that it stays in straight motion for the entire duration of observation. In this case no first turning point is observed and this event of a long, single step is instead described by  $s(\mathbf{x}|t,t_a)$ , which is the conditional probability that a walker that has aged for  $t_a$  performs a step of duration longer than t such that he is at  $\mathbf{x}$  at time t.

The transport equation for the PDF therefore has two terms corresponding to these cases:

$$p(\mathbf{x}|t,t_a) = \int_{\mathbb{R}^d} d^d x' \int_{\mathbb{R}^d} d^d x'' \int_0^t dt' \int_0^{t-t'} dt'' F(\mathbf{x}',t'|t_a) C(\mathbf{x}'',t'') r(\mathbf{x} - \mathbf{x}' - \mathbf{x}''|t - t' - t'')$$

$$+ s(\mathbf{x}|t,t_a). \tag{2.37}$$

The second term captures the contribution from the single step case while the double convolution describes a particle having its first turning point at t', then performing a series of completed steps for the duration t'' and then being found at observation time t in a final, incomplete step of duration t - t' - t'' or longer, as shown in the upper picture of figure (2.4).

Again using the convolution property of the Fourier and the Laplace transform, (2.30) and (2.30), we obtain the a closed expression for  $p(\mathbf{k}|s, t_a)$ :

$$p(\mathbf{k}|s, t_a) = F(\mathbf{k}, s|t_a)C(\mathbf{k}, s)r(\mathbf{k}|s) + s(\mathbf{k}|s, t_a). \tag{2.38}$$

### 3. Methodology

#### 3.1 Calculating the mean squared displacement

For the calculation of the MSD I will concentrate on the one-dimensional case, as this simplifies the calculations and generalizations to higher dimensions are clear, as the PDF of the process (2.7) is isotropic and the normalization takes care of the angular integral.

The one-dimensional MSD  $\langle x^2 \rangle(t)$  is defined via the integral

$$\langle x^2 \rangle(t) = \int_{\mathbb{R}} x^2 \psi(x, t) dx,$$
 (3.1)

which is closely related to the Fourier Laplace transform of the PDF for the process, as we can see when we expand it for small  $\mathbf{k}$ :

$$p(\mathbf{k}|s) = \int_{\mathbb{R}} e^{ikx} p(x|s) dx \tag{3.2}$$

$$= \int_{\mathbb{R}} p(x|s)dx + ik \int_{\mathbb{R}} xp(x|s)dx - \frac{k^2}{2} \int_{\mathbb{R}} x^2 p(x|s)dx$$
 (3.3)

$$=1-\frac{k^2}{2}\langle x^2\rangle(s)+\dots , \qquad (3.4)$$

where I used that the PDF is normalized to one and that the first moment of an isotropic process vanishes. This implies

$$\langle x^2 \rangle(s) = -\left[\frac{\partial^2}{\partial k^2} p(k|s)\right]_{k=0},$$
 (3.5)

which allows me to calculate the MSD directly without knowledge of the full PDF and then transforming it back into the time domain.

For the ordinary or non-aged case we can use expression (2.35) for the PDF in the Fourier Laplace domain:

$$p(k|s) = C(k,s)r(k|s). \tag{3.6}$$

We can expand C and r similarly to what we did for the PDF resulting in in

$$r(k|s) = r_0(s) - \frac{1}{2}k^2r_2(s) + o(k^2)$$
(3.7)

$$C(k,s) = C_0(s) - \frac{1}{2}k^2C_2(s) + o(k^2).$$
(3.8)

Here we see that the first moments vanish again and I introduced the new notation

$$r_0(s) = r(k=0|s)$$
 and  $r_2(s) = \left[\frac{\partial^2}{\partial k^2} r(k|s)\right]_{k=0}^{\infty}$ .

Inserting these expression we find for the PDF

$$p(k|s) = C_0(s)r_0(s) - \frac{k^2}{2} \left[ C_0(s)r_2(s) + C_2(s)r_0(s) \right] + o(k^2), \tag{3.9}$$

and therefore in the ordinary case the MSD is given by

$$\langle x^2 \rangle(s) = C_0(s)r_2(s) + C_2(s)r_0(s). \tag{3.10}$$

For the aged case we start from the result found in (2.38),

$$p(\mathbf{k}|s, t_a) = F(\mathbf{k}, s|t_a)C(\mathbf{k}, s)r(\mathbf{k}|s) + s(\mathbf{k}|s, t_a), \tag{3.11}$$

and use similar expansions for the transforms of the single step density and the first step density:

$$s(k|s,t_a) = s_0(s,t_a) - \frac{1}{2}k^2s_2(s,t_a) + o(k^2)$$
(3.12)

$$F(k, s|t_a) = F_0(s|t_a) - \frac{1}{2}k^2F_2(s|t_a) + o(k^2).$$
(3.13)

Thus we find for the PDF

$$p(k|s) = F_0(s|t_a)C_0(s)r_0(s) + s_0(s,t_a) - \frac{k^2}{2}s_2(s,t_a)$$
$$-\frac{k^2}{2}\left[F_0(s|t_a)C_0(s)r_2(s) + F_0(s|t_a)C_2(s)r_0(s) + F_2(s|t_a)C_0(s)r_0(s)\right] + o(k^2).$$
(3.14)

Therefore the MSD for the aged case reads

$$\langle x^2 \rangle(s) = F_0(s|t_a)C_0(s)r_2(s) + F_0(s|t_a)C_2(s)r_0(s) + F_2(s|t_a)C_0(s)r_0(s) + s_2(s,t_a).$$
(3.15)

To extract the asymptotic results from these formulas we need to look at the  $t \to \infty$  case, which corresponds to the  $s \to 0$  case in the Laplace domain.

The general strategy is therefore to find the expressions for  $C_0, F_0, r_0, C_2, F_2, r_2$  in the Laplace domain to leading order in s, insert them into the respective formulas for the MSD and transform back into the time domain using the Tauberian theorem. As  $s_2$  does not enter inside a product, it is not necessary to transform it and it can be calculated directly in the time domain.

#### 3.2 Finding the probability density function

#### 3.3 Numerical simulation of the model

Numerical simulations can be used to supplement and support analytical computations by giving insight into the qualitative structure of the process, sharpening understanding of the model and giving a method of testing the results. Furthermore simulations allow investigation of regimes where analytical computations fail.

In general there are two possible approaches for the simulation of a Lévy walk model: On the one hand a direct simulation of the process, where I randomly generate step durations and directions for a large ensemble of walkers and record their positions; or on the other hand a description via a suitable Langevin equation, which has been shown to be equivalent to a Lévy walk. I decided for the former approach as it keeps closer to the model and avoids potential numerical instabilities that can appear during the integration of differential equation. It is also not entirely clear how the generalization of the Lévy walk studied in this paper could be reflected in a Langevin equation.

The two main quantities of interest in this thesis are the MSD and the PDF of the generalized Lévy walk, which can be obtained from an ensemble of simulated walkers via averaging and creating histograms respectively. The simulation was implemented in one dimension similarly to the analytical computation, as this captures most of the behavior in an isotropic walk.

When performing the simulation duration of the walk and the size of the ensemble have the biggest impact on computation times, where the second factor is of special importance for processes with power law distributions such as Lévy walks, because here the walk is often dominated by rare events which are only captured with sufficiently large ensembles.

To address this issue I use the independence of the different walkers to parallelize the computation and perform it on the available graphics cards (GPUs) using NVIDIAs C++ extension CUDA. The university computers are equipped with Quadro K4000 GPUs, that have 768 cores each. This is a far than greater number of cores than available on processor (CPU), which is usually less than ten, and thus allows for far greater parallelization, resulting in a considerable speedup of the simulation.

Possible hurdles to this approach are the latency in the data transfer between working memory and GPU, which can slow down performance, and the limited memory on the GPU (3GB). However by limiting the walker positions I save to selected measurement times and reducing communication between GPU and CPU to a minimum it was possible to simulate large ensembles of 10<sup>9</sup> particle in a few hours.

Another aspect that should be addressed is the generation of pseudo random numbers for the creation of the steps for the simulation. As these numbers are not truly random, i.e. not completely uncorrelated, they can, depending on the quality of the number generator, leave statistical artifacts that falsify the simulation results. To minimize this risk I rely on the cuRAND library, which implements a version of the Xorshift algorithm [13]. The documentation guarantees a period greater than  $2^{190}$  for each independently seeded sequence (i.e. each simulation), and each thread has an offset of  $2^{67}$  in this sequence. At roughly  $10^9$  threads that each simulate a random walker with a step number lower than  $10^7$  I am more than ten orders of magnitude away from reaching the period of the random number sequence, which leaves little risk that statistical artifacts influenced the results.

quantify this?

is it?

# 4. Analytical Calculations

## 5. Results and Discussion

# 6. Conclusions

### **Bibliography**

- [1] RICHARDSON, Lewis F.: Atmospheric diffusion shown on a distance-neighbour graph. In: Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character 110 (1926), Nr. 756, S. 709–737
- [2] Zaburdaev, V; Denisov, S; Klafter, J: Lévy walks. In: Reviews of Modern Physics 87 (2015), Nr. 2, S. 483
- [3] Shlesinger, MF; West, BJ; Klafter, Joseph: Lévy dynamics of enhanced diffusion: Application to turbulence. In: *Physical Review Letters* 58 (1987), Nr. 11, S. 1100
- [4] Korobkova, Ekaterina; Emonet, Thierry; Vilar, Jose M.; Shimizu, Thomas S.; Cluzel, Philippe: From molecular noise to behavioural variability in a single bacterium. In: *Nature* 428 (2004), Nr. 6982, S. 574
- [5] Albers, Tony; Radons, Günter: Exact results for the nonergodicity of ddimensional generalized levy walks. In: *Physical review letters* 120 (2018), Nr. 10, S. 104501
- [6] SCHULZ-BALDES, Hermann: Anomalous Drude Model. In: Physical review letters 78 (1997), Nr. 11, S. 2176
- [7] Benkadda, Sadruddin; Zaslavsky, George M.: Chaos, Kinetics and Nonlinear Dynamics in Fluids and Plasmas: Proceedings of a Workshop Held in Carry-Le Rouet, France, 16–21 June 1997. Bd. 511. Springer Science & Business Media, 1998
- [8] Barkai, Eli: Aging in Subdiffusion Generated by a Deterministic Dynamical System. In: *Phys. Rev. Lett.* 90 (2003), Mar, 104101. http://dx.doi.org/10.1103/PhysRevLett.90.104101. DOI 10.1103/PhysRevLett.90.104101
- [9] Barkai, Eli; Cheng, Yuan-Chung: Aging continuous time random walks. In: *The Journal of chemical physics* 118 (2003), Nr. 14, S. 6167–6178
- [10] Klages, Rainer; Radons, Günter; Sokolov, Igor M.: *Anomalous transport*. Wiley Online Library, 2008
- [11] BROKMANN, X.; HERMIER, J.-P.; MESSIN, G.; DESBIOLLES, P.; BOUCHAUD, J.-P.; DAHAN, M.: Statistical Aging and Nonergodicity in the Fluorescence of Single Nanocrystals. In: *Phys. Rev. Lett.* 90 (2003), Mar, 120601. http://dx.doi.org/10.1103/PhysRevLett.90.120601. – DOI 10.1103/PhysRevLett.90.120601

- [12] Klafter, Joseph ; Sokolov, Igor M.: First steps in random walks: from tools to applications. Oxford University Press, 2011
- [13] MARSAGLIA, George u. a.: Xorshift rngs. In: Journal of Statistical Software 8 (2003), Nr. 14, S. 1–6

# Selbstständigkeitserklärung

· · · · · · · · · · · · · · · · · · ·	ass ich die vorliegende Arbeit selbstandig verfasst und enen Quellen und Hilfsmittel verwendet habe.	кеп
Ort, Datum	Unterschrift	